Optimizing Perchlorate Bioremediation: Analyzing the Role of Fe-S Complexes and Sulfates in pcrABCD Protein Activity Through Novel Docking Simulations

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Perchlorates are environmental pollutants that damage the human thyroid gland, stemming from military operations, rocket propellants, and fertilizer runoff. They also compose 0.5-1% of Martian soil. Two substances often found alongside perchlorates on Earth and Mars are iron-sulfur (Fe-S) complexes and sulfates. These substances enter the environment through mineral dissolution/industrial waste and naturally form on Mars. In some bacteria, the pcrABCD genes code for perchlorate reductase, enabling them to degrade perchlorates. They also have the Cld gene which allows them to degrade chlorites, a toxic byproduct, through chlorite dismutase. The previous year's study modeled and verified these proteins' structures. Then, it found through protein-ligand docking simulations that the pcrABCD proteins could degrade perchlorates effectively, and the Cld protein could degrade chlorites effectively. Thus, bacteria with the pcrABCD genes were projected to be a sustainable and effective method of perchlorate bioremediation. However, the previous study did not analyze the effects of Fe-S complexes and sulfates that could alter the enzyme's activity. This study analyzed the effects of Fe-S complexes and sulfates on perchlorate/chlorite binding affinity through novel docking simulations using Autodock Vina between the pcrA protein and perchlorates, or between the Cld protein and chlorites, alongside Fe-S complexes and sulfates. The study found that the distances between the sulfate/Fe-S complex and perchlorate/chlorite binding sites were statistically significant, and perchlorates/chlorites bound well to the proteins. This study thus provides crucial evidence confirming the viability of bacterial proteins in perchlorate bioremediation even in the presence of sulfates/Fe-S complexes.

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